Supporting Information: Electronic Structures of Pd^{II} Dimers

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Figure S1. Cyclic voltammograms of **1-4** in CH_2Cl_2.

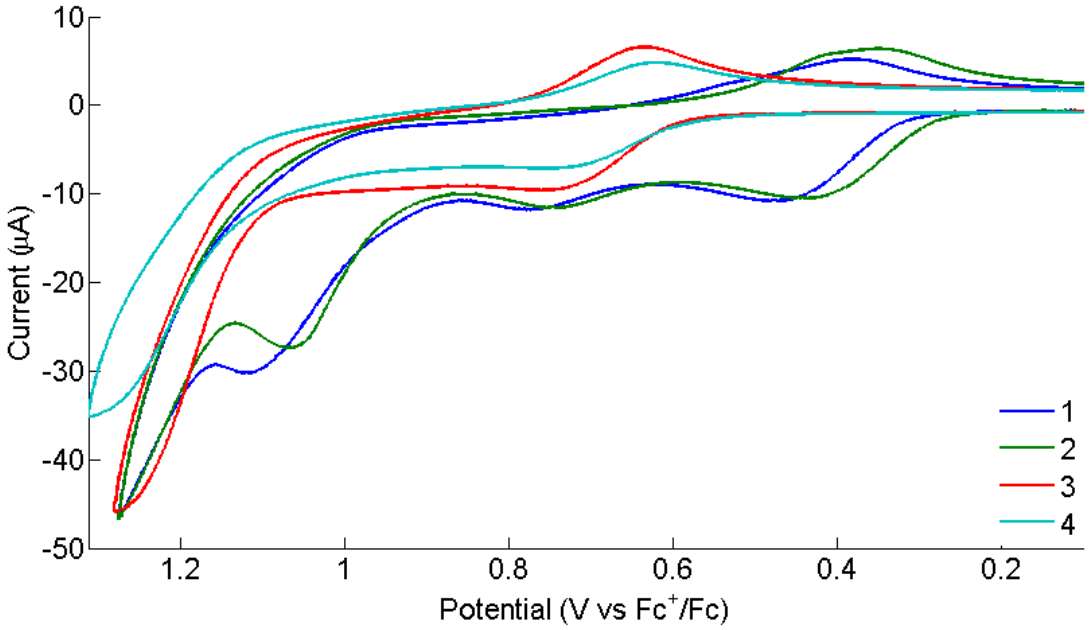
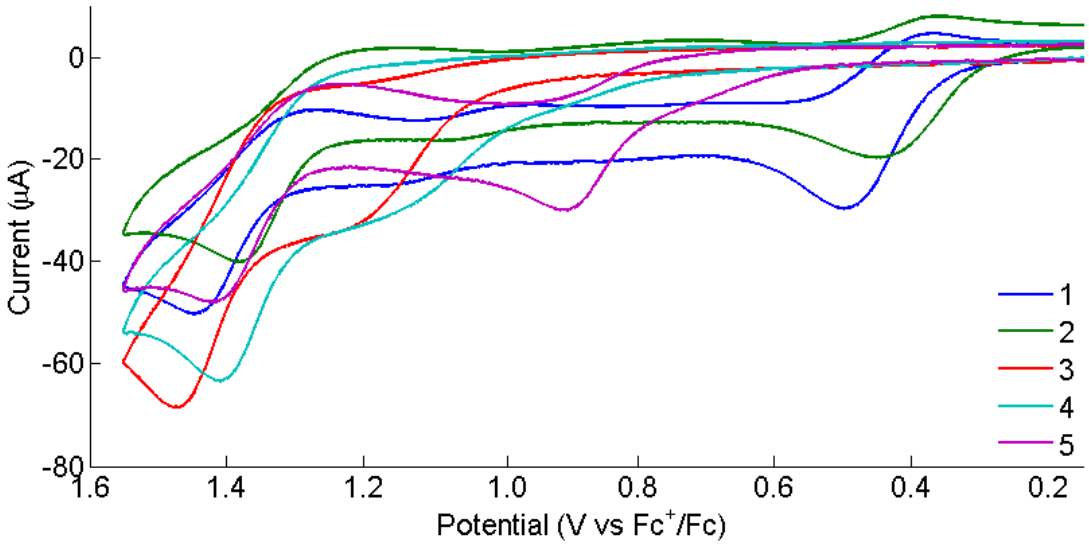


Figure S2. Cyclic voltammograms of **1-5** in MeCN.



Photophysics:

Figure S3. Steady-state emission spectra of **1-4**, 77 K, λ_{ex} = 355 nm.

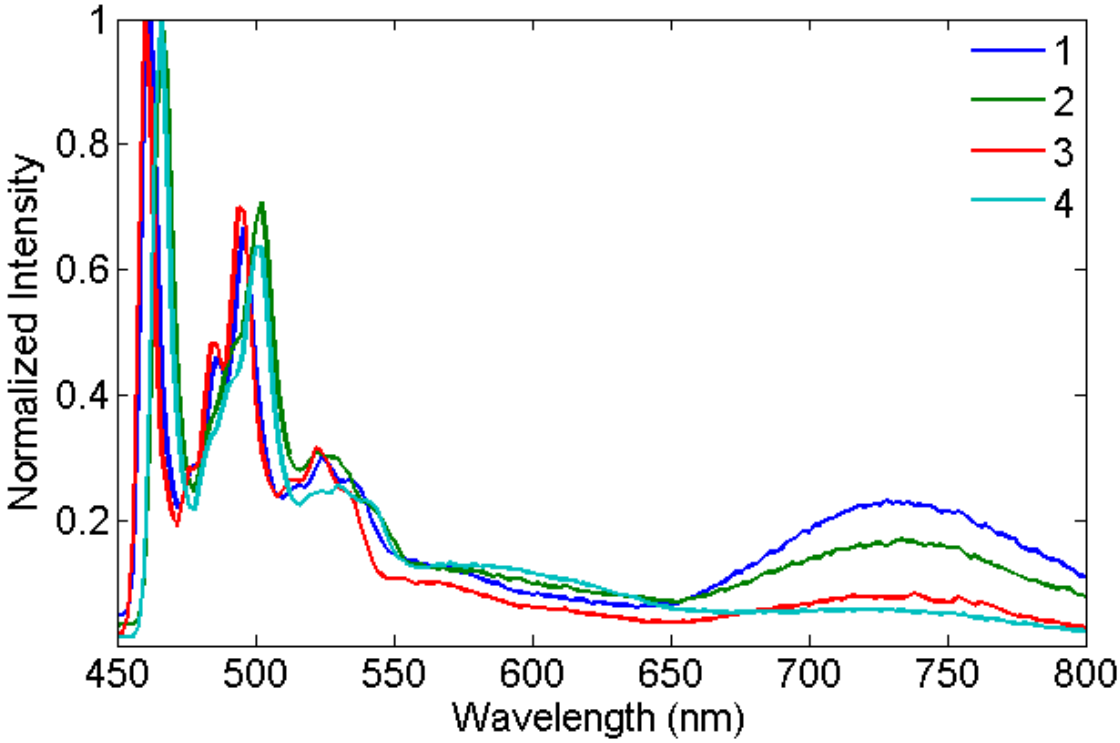


Figure S4. Steady-state emission spectra of **1-5**, 77 K, λ_{ex} = 355 nm.

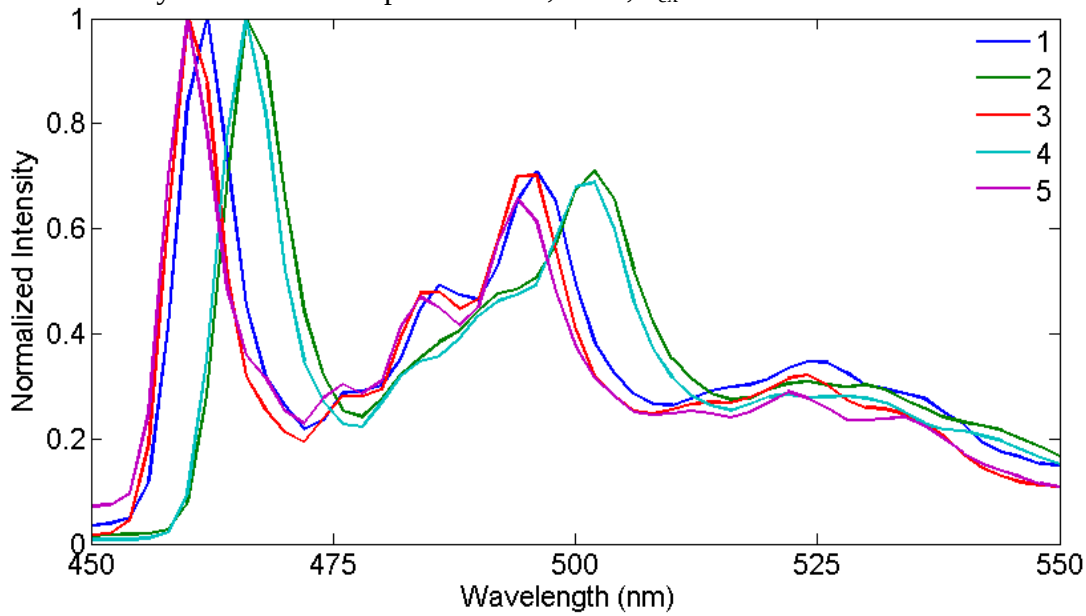


Figure S5. Excitation spectra of **1-4**, 77 K, λ_{em} = 460 nm.

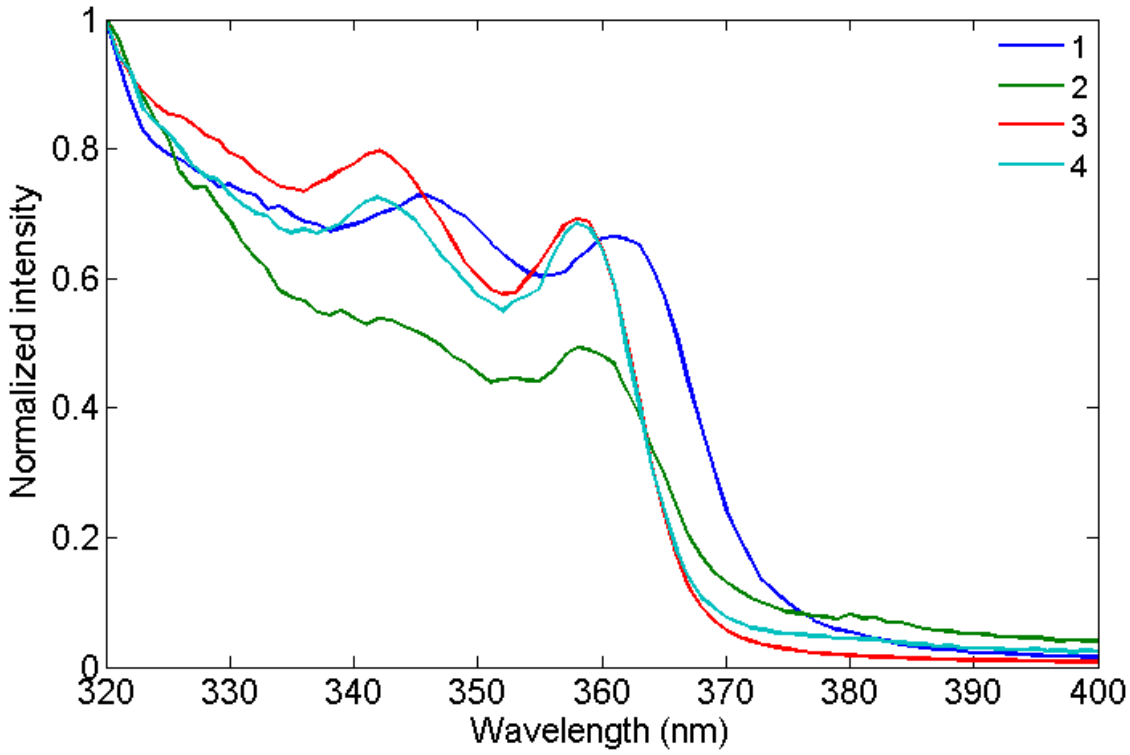
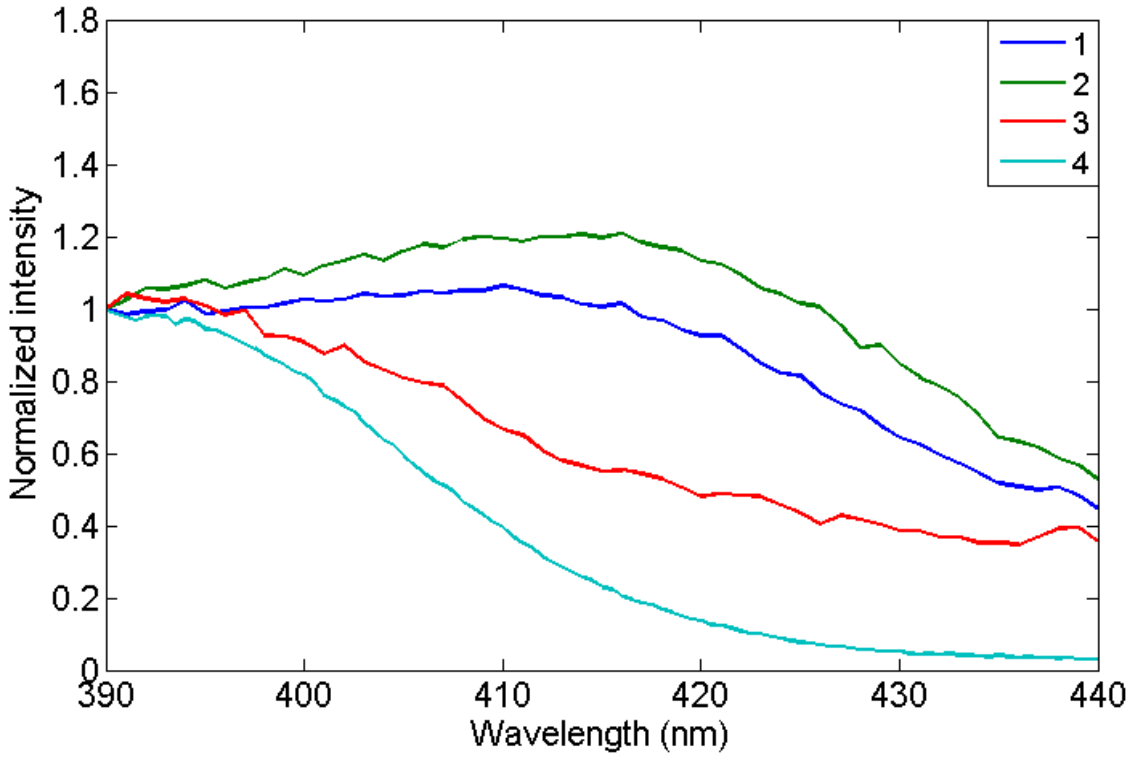
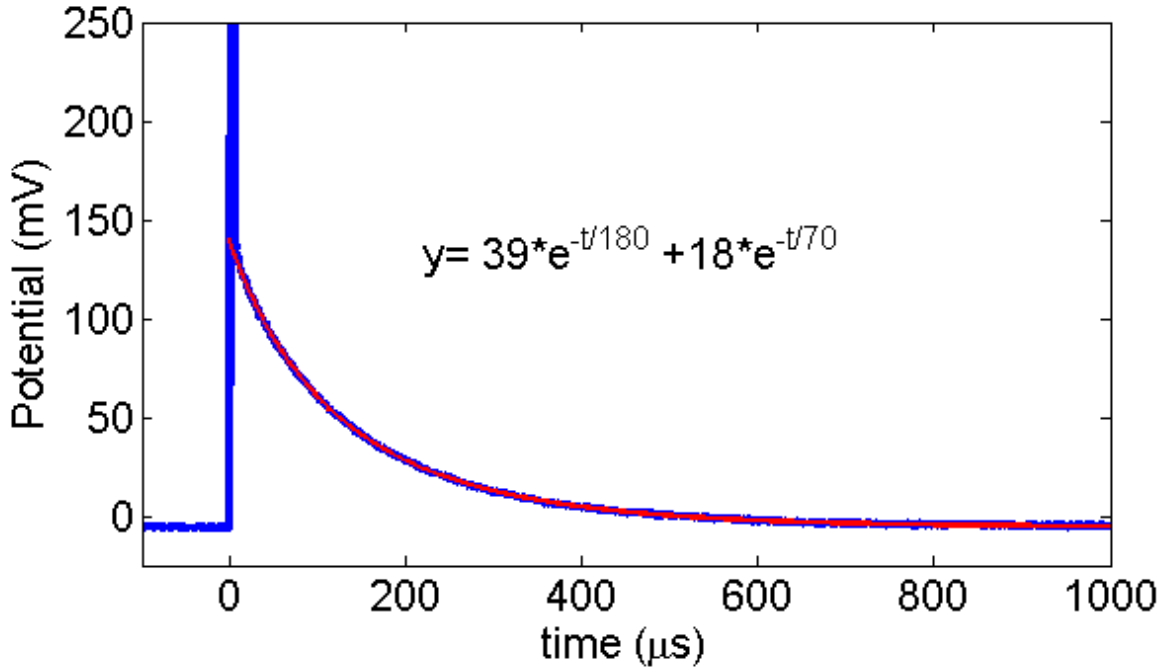


Figure S6. Excitation spectra of **1-4**, 77 K, λ_{em} = 790 nm.



Time-resolved data were collected on samples in MTHF glasses at 77 K. All lifetimes are reported in microseconds and the prefactors reflect the intensity of the signal in mV. The short-lived fluorescence components observed at 460 nm were not fit as their lifetimes exceeded the limits of the instrument ($\tau < 20$ ns).

Figure S7. Fitted lifetime of **1**.
a) 460 nm



b) 720 nm

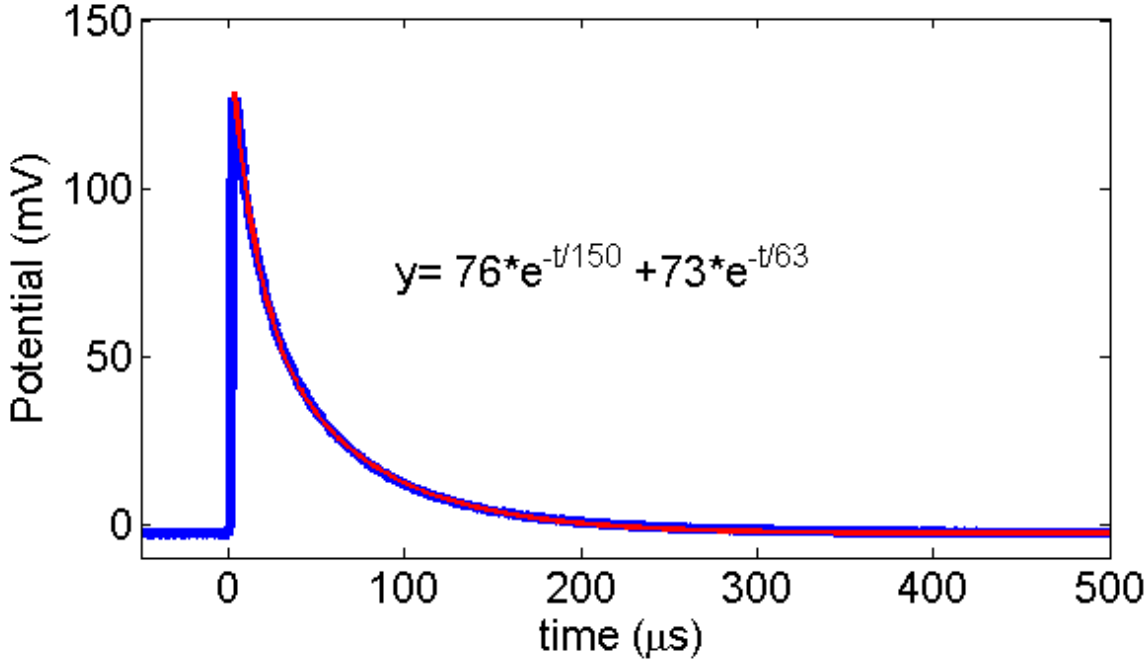
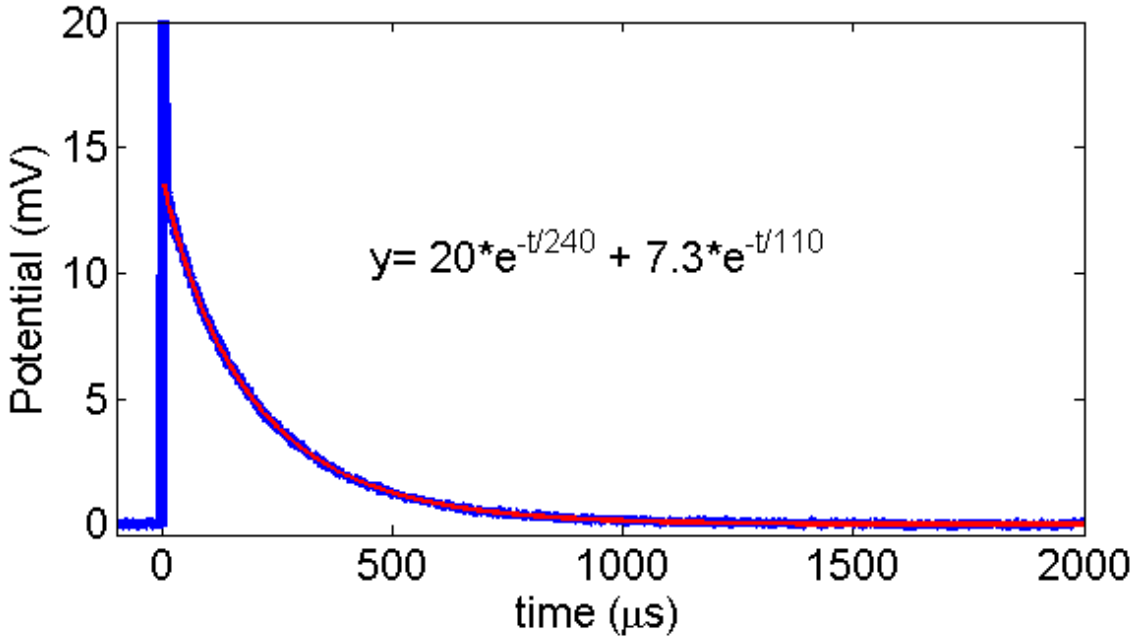


Figure S8. Fitted lifetime of **2**.
a) 460 nm



b) 720 nm

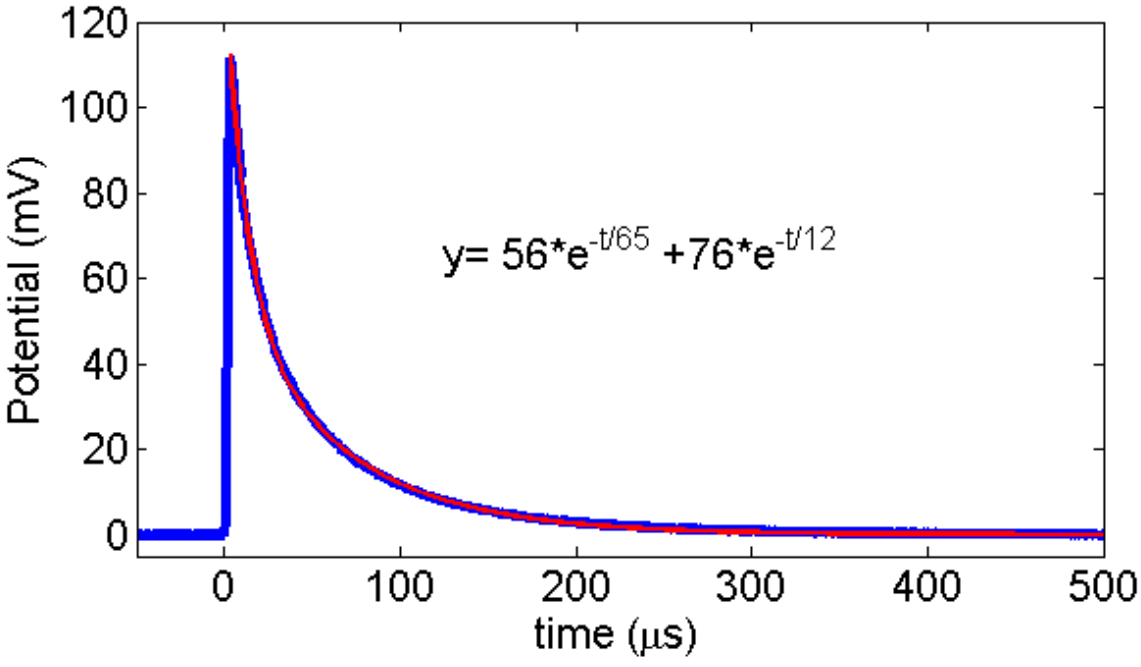
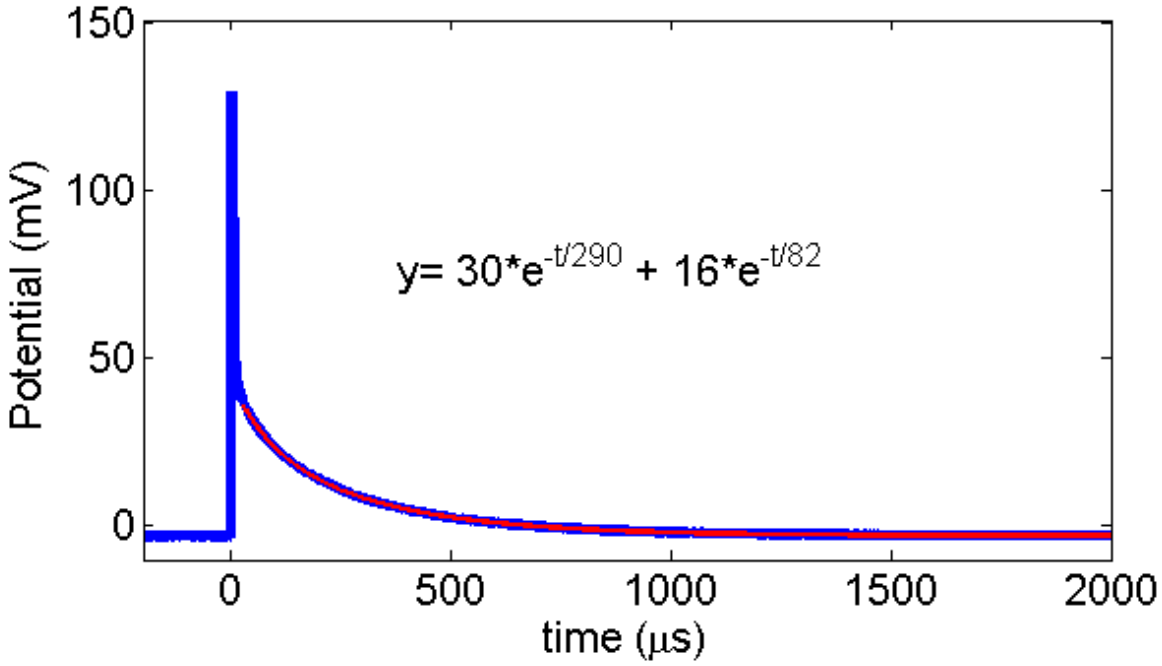


Figure S9. Fitted lifetime of **3**.
a) 460 nm



b) 720 nm

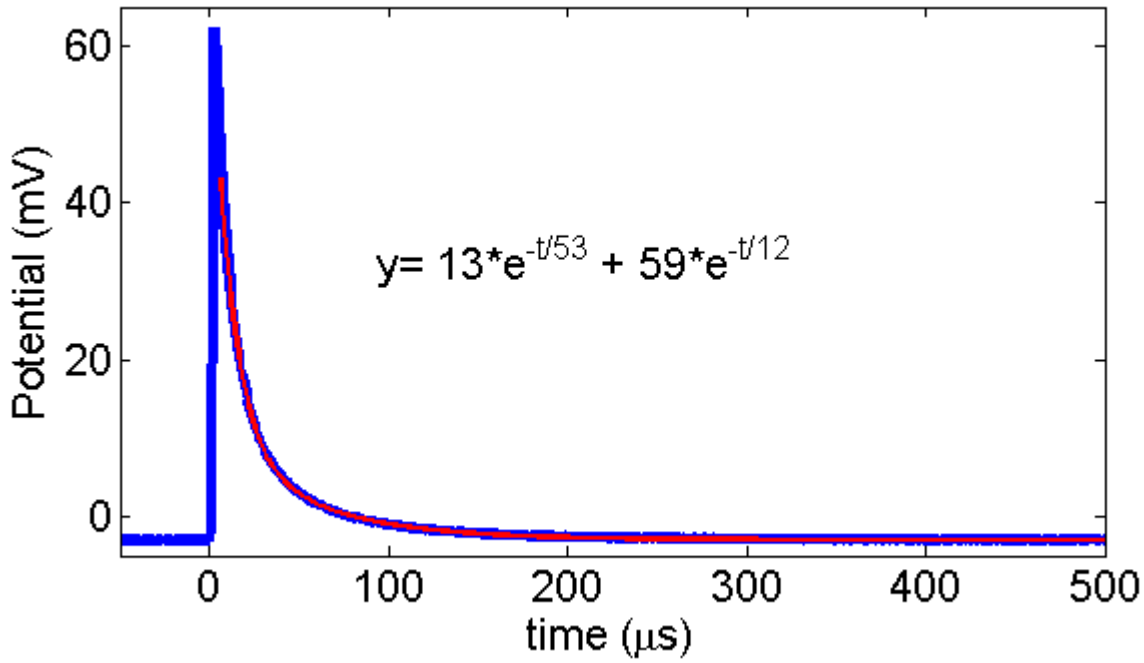
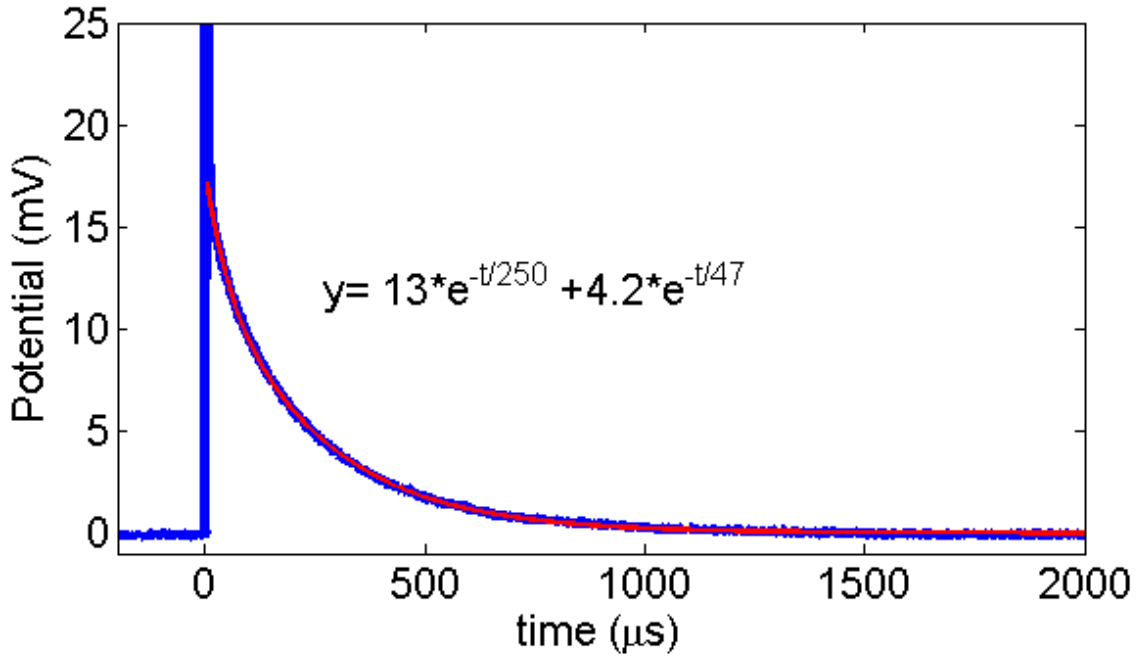


Figure S10. Fitted lifetime of **4**.
a) 460 nm



b) 720 nm

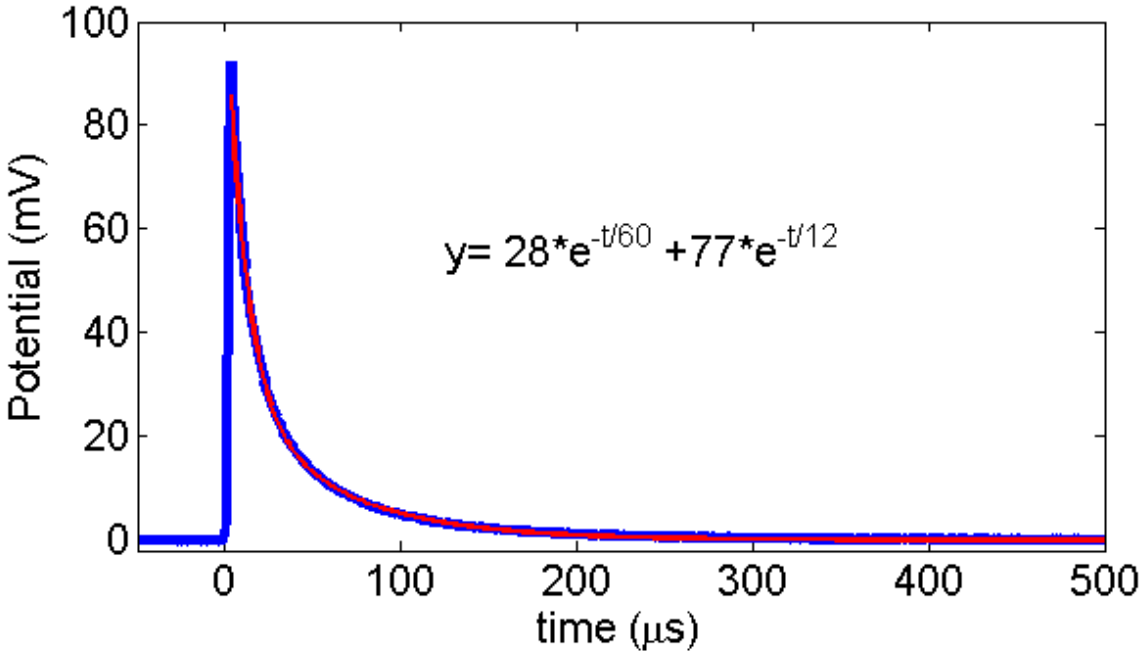
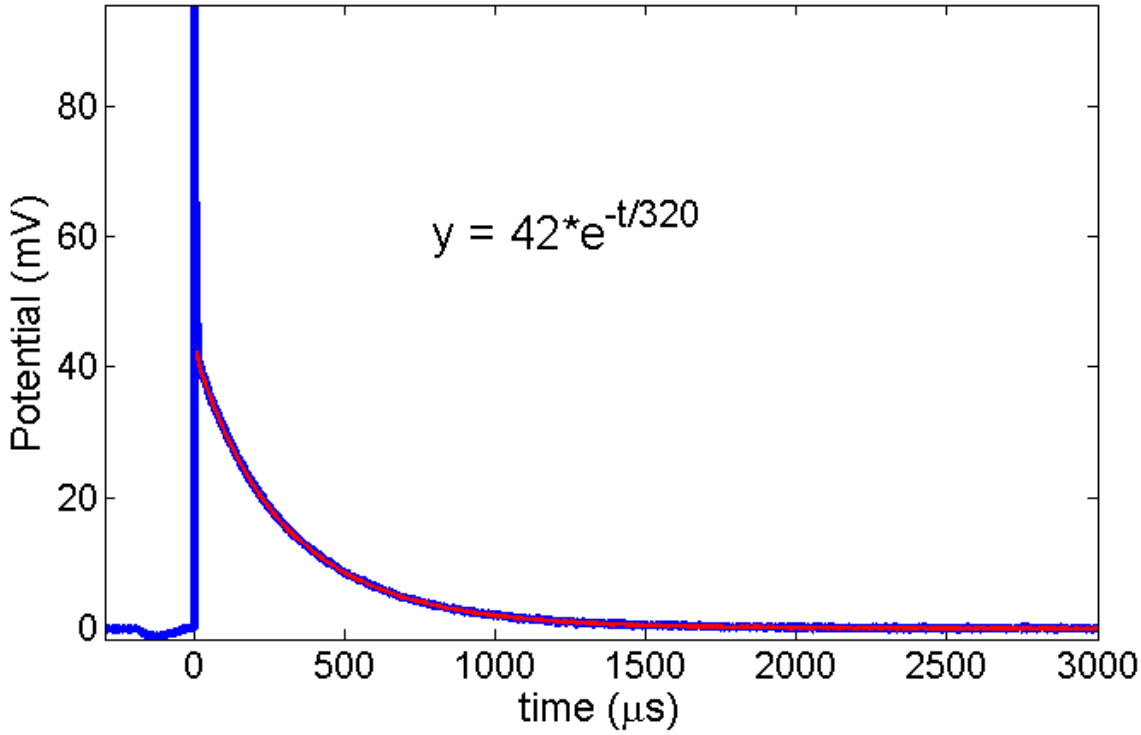


Figure S11. Fitted lifetime of **5**.

a) 460 nm

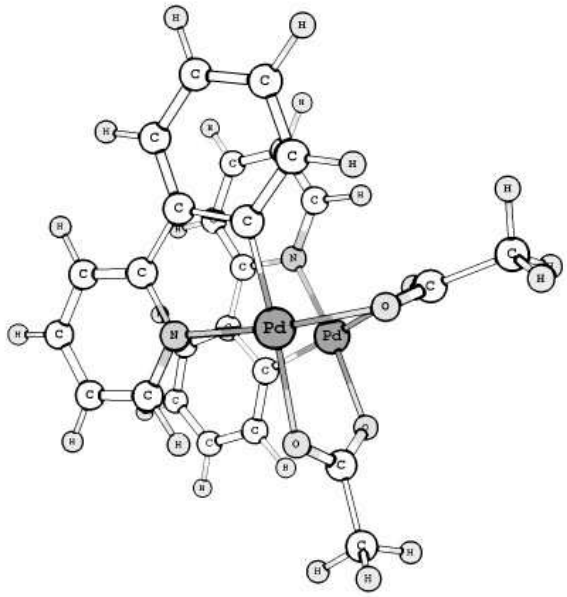


Density Functional Theory
XYZ coordinates of optimized structures

Compound 1

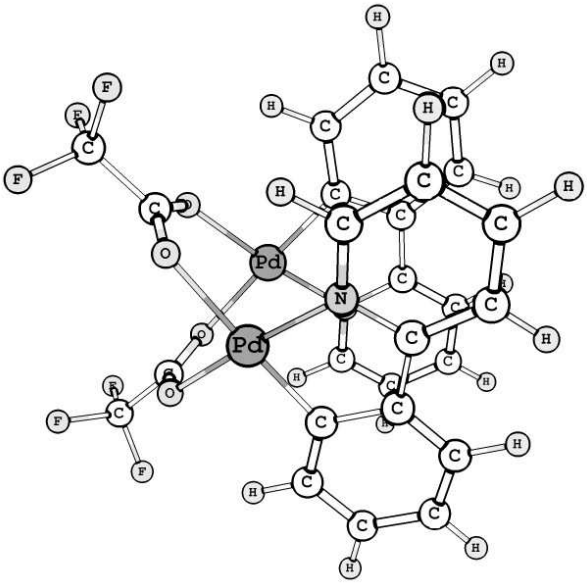
Atom	X	Y	Z (Angstrom)
1.Pd	8.385247000	11.197963000	6.669546000
2.Pd	9.030302000	13.116676000	4.793108000
3.H	7.226868000	15.674246000	8.160614000
4.H	5.849269000	14.564166000	8.367851000
5.H	5.965256000	15.631425000	6.907193000
6.H	4.692633000	10.550621000	4.220326000
7.H	5.846351000	9.967429000	2.991907000
8.H	5.205495000	11.618824000	2.848969000
9.N	7.588036000	12.917008000	7.557162000
10.N	7.670811000	14.245764000	5.738533000
11.N	6.728976000	10.934525000	5.572936000
12.N	7.531875000	12.055702000	3.790250000
13.O	10.096131000	11.293389000	7.639741000
14.O	10.513646000	12.106868000	3.982410000
15.C	10.407168000	12.281355000	8.476041000
16.C	11.667733000	12.399836000	9.022327000
17.C	12.631934000	11.463806000	8.681583000
18.C	12.304223000	10.443654000	7.813192000
19.C	11.021323000	10.367616000	7.291371000
20.C	10.523333000	9.384588000	6.364011000
21.C	11.260064000	8.309832000	5.880076000
22.C	10.679085000	7.417201000	4.999858000
23.C	9.357150000	7.598103000	4.612975000
24.C	8.618778000	8.671685000	5.088421000
25.C	9.190525000	9.585746000	5.961000000
26.C	10.332428000	11.089221000	3.143332000
27.C	11.383935000	10.308539000	2.711778000
28.C	12.659048000	10.593281000	3.175600000
29.C	12.840048000	11.646995000	4.046859000
30.C	11.750056000	12.405325000	4.447987000
31.C	11.762984000	13.522845000	5.356602000
32.C	12.906359000	14.050620000	5.944986000
33.C	12.806014000	15.137424000	6.792347000
34.C	11.560141000	15.698507000	7.043128000
35.C	10.415156000	15.172839000	6.463027000
36.C	10.495565000	14.072791000	5.622022000
37.C	6.682182000	11.334052000	4.371221000
38.C	5.521825000	10.851017000	3.567388000
39.C	7.309342000	13.964157000	6.920186000
40.C	6.520830000	15.015690000	7.626387000
41.H	9.595660000	12.985407000	8.683326000
42.H	11.886847000	13.226922000	9.700075000
43.H	13.641951000	11.534636000	9.093600000
44.H	13.040292000	9.690711000	7.520360000
45.H	12.296908000	8.166070000	6.202561000
46.H	11.250939000	6.566071000	4.622411000
47.H	8.889787000	6.879856000	3.932398000
48.H	7.571256000	8.792834000	4.792302000
49.H	9.295532000	10.920575000	2.837362000
50.H	11.195419000	9.479416000	2.027334000
51.H	13.511693000	9.987801000	2.857341000
52.H	13.830529000	11.896981000	4.435362000
53.H	13.886348000	13.610990000	5.730516000
54.H	13.702593000	15.562326000	7.250145000
55.H	11.482026000	16.570972000	7.699029000

56.H 9.440599000 15.636194000 6.651016000



Atom	X	Y	Z (Angstrom)
1.Pd	8.405940	11.170688	6.682973
2.Pd	9.001517	13.190823	4.756391
3.F	7.079164	15.977153	8.120844
4.F	5.603517	14.470104	8.594779
5.F	5.470082	15.558200	6.735815
6.F	4.597094	10.168097	4.230325
7.F	5.853791	10.236662	2.468456
8.F	4.717854	11.983236	3.061309
9.O	7.405606	12.881381	7.530108
10.O	7.696986	14.350726	5.819304
11.O	6.788729	10.851505	5.461157
12.O	7.340858	12.278520	3.779528
13.N	10.061647	11.326680	7.788633
14.N	10.394366	12.100990	3.824211
15.C	10.269199	12.267519	8.712638
16.C	11.471881	12.390683	9.380600
17.C	12.501210	11.512787	9.079994
18.C	12.284293	10.537067	8.127796
19.C	11.054715	10.449032	7.486170
20.C	10.685090	9.477863	6.482796
21.C	11.517303	8.467413	5.997072
22.C	11.048383	7.584143	5.042243
23.C	9.745747	7.703454	4.575671
24.C	8.911619	8.709194	5.046605
25.C	9.371637	9.614885	5.992632
26.C	10.162554	11.184600	2.881609
27.C	11.158434	10.345477	2.421651
28.C	12.435232	10.456151	2.948014
29.C	12.696740	11.467241	3.847759
30.C	11.659127	12.276938	4.293235
31.C	11.778833	13.334581	5.271905
32.C	12.979175	13.743021	5.852454
33.C	12.992056	14.798155	6.747314
34.C	11.804097	15.452756	7.051938
35.C	10.598204	15.036233	6.492729
36.C	10.571473	13.970067	5.606973
37.C	6.640393	11.420865	4.352452
38.C	5.418459	10.948421	3.529983

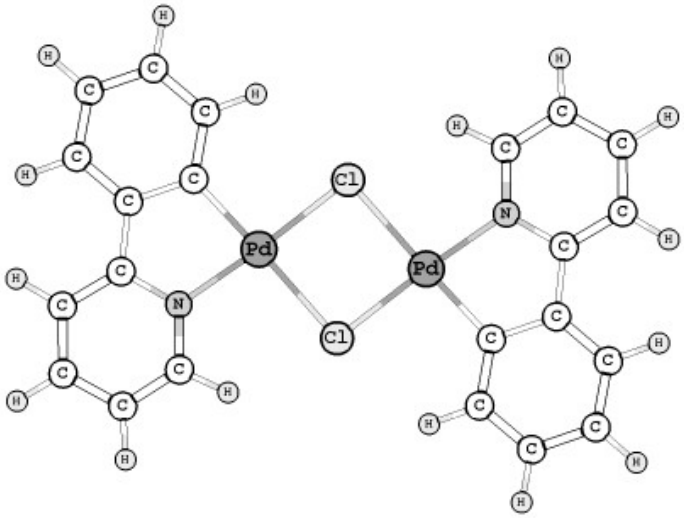
39.C	7.223331	13.948384	6.913065
40.C	6.314490	14.995154	7.600201
41.H	9.435697	12.945347	8.923437
42.H	11.584648	13.173704	10.134477
43.H	13.462235	11.596472	9.598608
44.H	13.058431	9.810716	7.863235
45.H	12.550079	8.359411	6.349619
46.H	11.694875	6.792211	4.651382
47.H	9.381634	6.999025	3.819931
48.H	7.888276	8.778246	4.662483
49.H	9.142531	11.112712	2.485189
50.H	10.938711	9.593410	1.659871
51.H	13.192187	9.725314	2.643267
52.H	13.704748	11.647066	4.232876
53.H	13.910029	13.234055	5.581135
54.H	13.929122	15.129747	7.205167
55.H	11.820920	16.310846	7.732551
56.H	9.665135	15.558403	6.733072



Compound 5

Atom	X	Y	Z (Angstrom)
1.Pd	0.565215	1.624528	0.000000
2.Pd	-0.565215	-1.624528	0.000000
3.Cl	1.552121	-0.459282	0.000000
4.Cl	-1.552121	0.459282	0.000000
5.N	-0.180573	3.466242	0.000000
6.C	2.248687	2.614696	0.000000
7.N	0.180573	-3.466242	0.000000
8.C	-2.248687	-2.614696	0.000000
9.C	1.961472	-5.034013	0.000000
10.H	3.039269	-5.212935	0.000000
11.C	-4.474231	-4.309272	0.000000
12.H	-5.351249	-4.962273	0.000000
13.C	1.486440	-3.739417	0.000000
14.H	2.152335	-2.870318	0.000000
15.C	-3.528805	-2.084979	0.000000
16.H	-3.669730	-0.999091	0.000000
17.C	-2.092763	-4.012308	0.000000
18.C	1.048811	-6.078819	0.000000
19.H	1.394187	-7.116874	0.000000

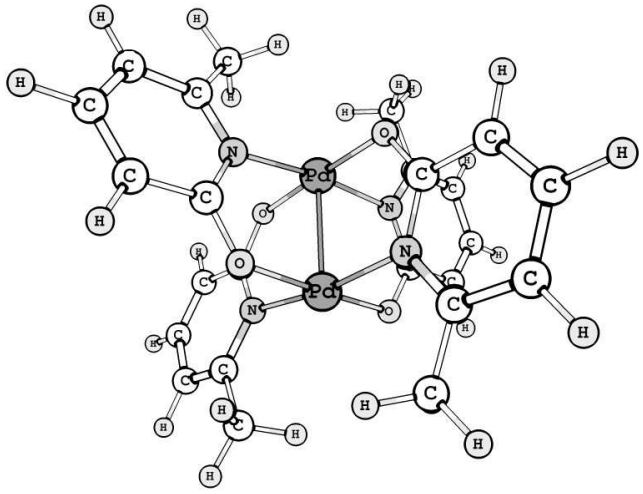
20.C	-4.631150	-2.928629	0.000000
21.H	-5.637524	-2.497499	0.000000
22.C	-3.203850	-4.851094	0.000000
23.H	-3.070473	-5.938546	0.000000
24.C	-0.729178	-4.472459	0.000000
25.C	-0.300665	-5.793332	0.000000
26.H	-1.047209	-6.592269	0.000000
27.C	0.729178	4.472459	0.000000
28.C	4.474231	4.309272	0.000000
29.H	5.351249	4.962273	0.000000
30.C	3.528805	2.084979	0.000000
31.H	3.669730	0.999091	0.000000
32.C	2.092763	4.012308	0.000000
33.C	0.300665	5.793332	0.000000
34.H	1.047209	6.592269	0.000000
35.C	-1.048811	6.078819	0.000000
36.H	-1.394187	7.116874	0.000000
37.C	-1.486440	3.739417	0.000000
38.H	-2.152335	2.870318	0.000000
39.C	-1.961472	5.034013	0.000000
40.H	-3.039269	5.212935	0.000000
41.C	4.631150	2.928629	0.000000
42.H	5.637524	2.497499	0.000000
43.C	3.203850	4.851094	0.000000
44.H	3.070473	5.938546	0.000000



Compound a

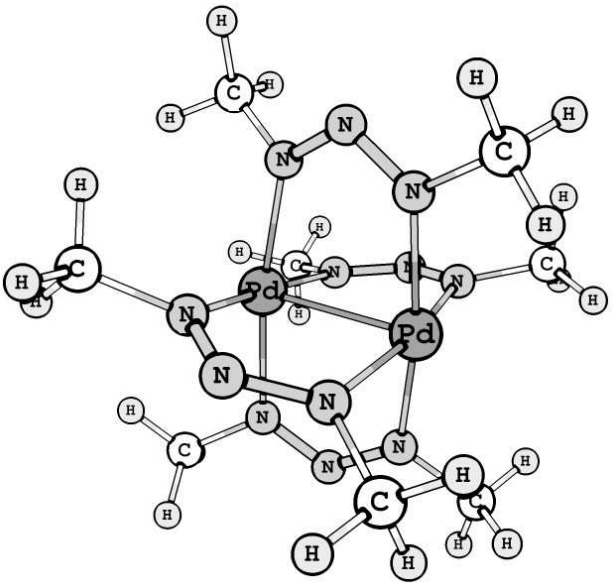
Atom	X	Y	Z (Angstrom)
1.Pd	1.264011	0.000000	0.000000
2.Pd	-1.264011	0.000000	0.000000
3.O	-1.225263	1.487607	-1.323780
4.O	1.225263	-1.487607	-1.323780
5.O	-1.225263	-1.487607	1.323780
6.O	1.225263	1.487607	1.323780
7.N	1.106177	1.332913	-1.518155
8.N	-1.106177	-1.332913	-1.518155
9.N	1.106177	-1.332913	1.518155
10.N	-1.106177	1.332913	1.518155
11.C	-0.108147	1.839090	-1.874483
12.C	-0.162808	2.805087	-2.903456
13.C	0.979195	3.194345	-3.545370
14.C	2.201988	2.632104	-3.182307

15.C	2.230322	1.704645	-2.166369
16.C	0.108147	-1.839090	-1.874483
17.C	0.162808	-2.805087	-2.903456
18.C	-0.979195	-3.194345	-3.545370
19.C	-2.201988	-2.632104	-3.182307
20.C	-2.230322	-1.704645	-2.166369
21.C	-0.108147	-1.839090	1.874483
22.C	-0.162808	-2.805087	2.903456
23.C	0.979195	-3.194345	3.545370
24.C	2.201988	-2.632104	3.182307
25.C	2.230322	-1.704645	2.166369
26.C	0.108147	1.839090	1.874483
27.C	0.162808	2.805087	2.903456
28.C	-0.979195	3.194345	3.545370
29.C	-2.201988	2.632104	3.182307
30.C	-2.230322	1.704645	2.166369
31.H	3.133162	-2.908137	3.682893
32.H	0.929753	-3.938703	4.346450
33.H	-1.149053	-3.202883	3.155006
34.H	-1.149053	3.202883	-3.155006
35.H	0.929753	3.938703	-4.346450
36.H	3.133162	2.908137	-3.682893
37.H	1.149053	-3.202883	-3.155006
38.H	-0.929753	-3.938703	-4.346450
39.H	-3.133162	-2.908137	-3.682893
40.H	1.149053	3.202883	3.155006
41.H	-0.929753	3.938703	4.346450
42.H	-3.133162	2.908137	3.682893
43.C	-3.485168	1.051892	1.729359
44.H	-4.341820	1.412962	2.315728
45.H	-3.666891	1.248293	0.658826
46.H	-3.395675	-0.042091	1.844057
47.C	-3.485168	-1.051892	-1.729359
48.H	-3.666891	-1.248293	-0.658826
49.H	-3.395675	0.042091	-1.844057
50.H	-4.341820	-1.412962	-2.315728
51.C	3.485168	1.051892	-1.729359
52.H	3.666891	1.248293	-0.658826
53.H	3.395675	-0.042091	-1.844057
54.H	4.341820	1.412962	-2.315728
55.C	3.485168	-1.051892	1.729359
56.H	4.341820	-1.412962	2.315728
57.H	3.666891	-1.248293	0.658826
58.H	3.395675	0.042091	1.844057



Compound b

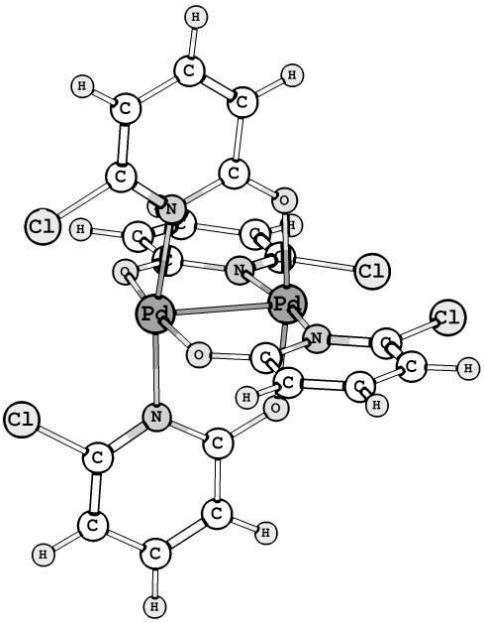
Atom	X	Y	Z (Angstrom)
1.N	-0.901383	-0.843200	-1.928842
2.N	-1.455852	1.646117	-0.660848
3.N	-0.510441	2.512108	-0.669410
4.N	0.679138	2.158806	-0.348112
5.N	0.195731	-0.641199	-2.561591
6.N	1.200875	-0.134247	-1.947277
7.N	1.474688	-1.708610	0.417026
8.N	0.509360	-2.507722	0.687152
9.N	-0.699977	-2.087168	0.632586
10.N	0.954379	0.574095	2.003745
11.N	-0.197052	0.645049	2.564231
12.N	-1.253273	0.406904	1.877040
13.Pd	1.241168	0.256988	0.031680
14.Pd	-1.241557	-0.256750	-0.027799
15.C	-1.889962	-1.556902	-2.678778
16.H	-2.011866	-2.581180	-2.282413
17.H	-2.866018	-1.051186	-2.599374
18.H	-1.585329	-1.620613	-3.737029
19.C	2.305836	0.194556	-2.795405
20.H	3.244122	-0.195407	-2.366277
21.H	2.148584	-0.231371	-3.800533
22.H	2.411009	1.292743	-2.885792
23.C	2.767593	-2.321853	0.407883
24.H	3.454829	-1.788540	1.087488
25.H	2.684791	-3.377011	0.715919
26.H	3.202011	-2.277836	-0.607207
27.C	-1.680177	-3.064692	1.003160
28.H	-1.219475	-3.855073	1.619643
29.H	-2.480614	-2.572719	1.581295
30.H	-2.145574	-3.528620	0.111765
31.C	-2.478700	0.692710	2.557952
32.H	-2.273903	0.940316	3.612598
33.H	-2.988452	1.551230	2.082988
34.H	-3.161142	-0.172430	2.503048
35.C	1.628492	3.229736	-0.324931
36.H	2.157985	3.239338	0.644683
37.H	2.388421	3.099952	-1.119259
38.H	1.112219	4.194357	-0.466376
39.C	2.059040	0.674846	2.907387
40.H	2.778564	1.432080	2.552648
41.H	1.698342	0.943521	3.914174
42.H	2.593259	-0.291741	2.967177
43.C	-2.709074	2.131916	-1.151566
44.H	-2.644863	3.217154	-1.336995
45.H	-2.974248	1.622070	-2.096114
46.H	-3.513208	1.925636	-0.423961



Compound c

Atom	X	Y	Z (Angstrom)
1.Pd	0.000000	0.000000	1.278900
2.Pd	0.000000	0.000000	-1.279033
3.Cl	1.745299	-0.789015	-3.719094
4.Cl	-1.745299	0.789015	-3.719094
5.Cl	-1.212059	-1.481652	3.719031
6.Cl	1.212059	1.481652	3.719031
7.O	0.995361	1.725601	-1.217104
8.O	1.656566	-1.106672	1.217015
9.O	-0.995361	-1.725601	-1.217104
10.O	-1.656566	1.106672	1.217015
11.N	1.124957	1.674332	1.120125
12.N	1.750835	-1.002252	-1.120230
13.N	-1.124957	-1.674332	1.120125
14.N	-1.750835	1.002252	-1.120230
15.C	1.403170	2.224100	-0.103992
16.C	2.179126	3.404169	-0.151221
17.C	2.649068	3.973573	0.998825
18.C	2.366170	3.393866	2.236028
19.C	1.604779	2.255095	2.225920
20.C	2.243420	-1.372135	0.103947
21.C	3.461917	-2.086177	0.151417
22.C	4.136120	-2.387733	-0.998449
23.C	3.626341	-1.992603	-2.235692
24.C	2.439062	-1.309376	-2.225889
25.C	-1.403170	-2.224100	-0.103992
26.C	-2.179126	-3.404169	-0.151221
27.C	-2.649068	-3.973573	0.998825
28.C	-2.366170	-3.393866	2.236028
29.C	-1.604779	-2.255095	2.225920
30.C	-2.243420	1.372135	0.103947
31.C	-3.461917	2.086177	0.151417
32.C	-4.136120	2.387733	-0.998449
33.C	-3.626341	1.992603	-2.235692
34.C	-2.439062	1.309376	-2.225889
35.H	-2.720832	-3.805724	3.181278
36.H	-3.252363	-4.885209	0.951427
37.H	-2.379322	-3.818696	-1.141799
38.H	2.379322	3.818696	-1.141799
39.H	3.252363	4.885209	0.951427

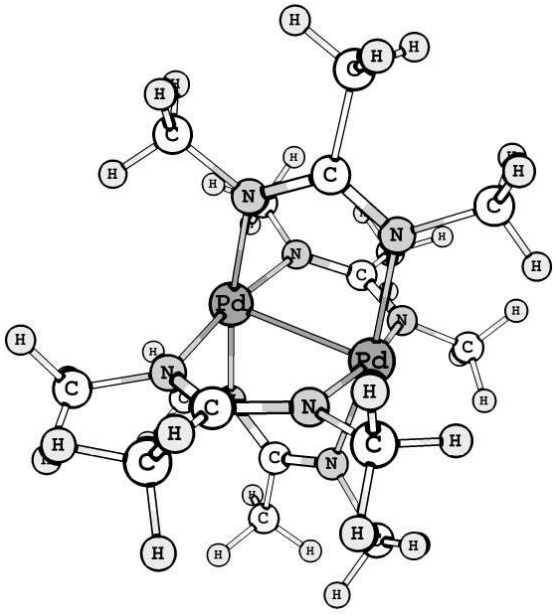
40.H	2.720832	3.805724	3.181278
41.H	3.824347	-2.369582	1.142113
42.H	5.081035	-2.937446	-0.950891
43.H	4.127527	-2.203768	-3.180743
44.H	-3.824347	2.369582	1.142113
45.H	-5.081035	2.937446	-0.950891
46.H	-4.127527	2.203768	-3.180743



Compound d

Atom	X	Y	Z (Angstrom)
1.Pd	-0.001348	-0.003657	-1.270687
2.Pd	0.000573	-0.003941	1.267476
3.N	-1.036355	1.715600	-1.134027
4.N	-0.626264	1.907213	1.145346
5.N	1.729089	1.019246	-1.141064
6.N	1.904947	0.633055	1.145825
7.N	1.018038	-1.735443	-1.148418
8.N	0.636992	-1.909764	1.140109
9.N	-1.728470	-1.027821	-1.147703
10.N	-1.903757	-0.648618	1.140689
11.C	-1.099463	2.391461	0.005070
12.C	2.384293	1.116877	0.008590
13.C	1.118346	-2.389397	0.002026
14.C	-2.401491	-1.089311	-0.007645
15.C	1.704187	-2.223450	-2.306451
16.H	1.410764	-3.256783	-2.582933
17.H	1.464704	-1.572046	-3.159078
18.H	2.809447	-2.216129	-2.191355
19.C	1.818500	-3.711965	-0.010995
20.H	1.235762	-4.467916	-0.566924
21.H	2.787672	-3.617539	-0.528904
22.H	2.005401	-4.090145	1.002388
23.C	0.546227	-2.723920	2.314232
24.H	0.269494	-3.773456	2.098339
25.H	1.484341	-2.737378	2.909236
26.H	-0.241227	-2.311187	2.964758
27.C	-2.724236	-0.618904	2.314371
28.H	-3.117937	-1.616621	2.597417
29.H	-2.119453	-0.251741	3.156002
30.H	-3.595795	0.063494	2.219062
31.C	-3.779544	-1.673733	0.000794

32.H	-3.776527	-2.695258	0.422266
33.H	-4.447102	-1.069237	0.635314
34.H	-4.209184	-1.719422	-1.008998
35.C	-2.191347	-1.709850	-2.318172
36.H	-2.656796	-2.689370	-2.097606
37.H	-2.921035	-1.115038	-2.908431
38.H	-1.327863	-1.902844	-2.974243
39.C	-0.544972	2.713629	2.326786
40.H	-1.527532	2.873557	2.817199
41.H	0.098536	2.196591	3.054660
42.H	-0.092417	3.709238	2.147246
43.C	-1.751860	3.738121	-0.016676
44.H	-2.847862	3.628600	-0.101418
45.H	-1.545186	4.309000	0.898093
46.H	-1.419337	4.326366	-0.887118
47.C	-1.710420	2.196124	-2.300527
48.H	-1.903418	1.345600	-2.973272
49.H	-2.685810	2.669795	-2.076799
50.H	-1.107806	2.933302	-2.873039
51.C	2.714127	0.553681	2.324620
52.H	2.283575	-0.210112	2.991321
53.H	3.758945	0.251975	2.118672
54.H	2.743525	1.504458	2.898379
55.C	3.706379	1.816912	-0.005057
56.H	4.452137	1.251626	-0.591686
57.H	3.603517	2.800989	-0.492869
58.H	4.101877	1.973982	1.006675
59.C	2.219944	1.704758	-2.298195
60.H	1.556753	1.484470	-3.146638
61.H	2.237104	2.808789	-2.173346
62.H	3.244734	1.392603	-2.586579

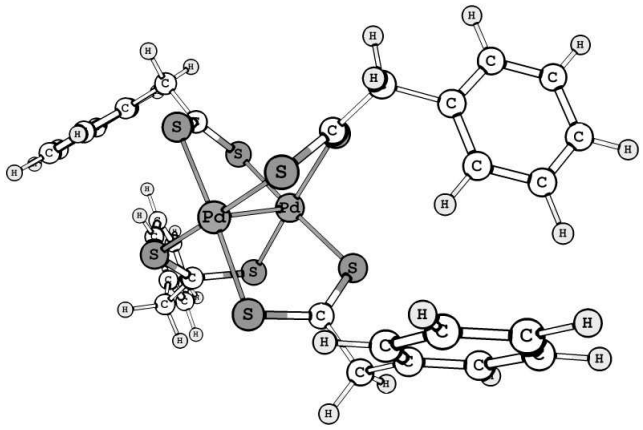


Compound e

Atom	X	Y	Z (Angstrom)
1.Pd	0.000000	0.000000	1.573542
2.Pd	0.000000	0.000000	-1.105541
3.S	-2.162553	-0.809085	1.644804

4.S	-0.841421	2.148563	1.659921
5.S	-1.579099	-1.677986	-1.201531
6.S	-1.693879	1.568707	-1.195281
7.C	-2.493975	-1.615868	0.207416
8.C	-1.707856	2.429906	0.241937
9.C	-3.786900	-2.376081	0.182077
10.C	-2.662375	3.586102	0.300922
11.C	-4.764056	-1.869729	-0.836420
12.C	-5.192383	-0.546668	-0.808590
13.C	-6.109088	-0.091250	-1.740781
14.C	-6.609120	-0.948584	-2.710077
15.C	-6.185605	-2.267471	-2.742936
16.C	-5.265331	-2.722210	-1.810980
17.C	-4.058525	3.137460	0.627641
18.C	-5.088255	3.344885	-0.280773
19.C	-6.381825	2.945644	0.016216
20.C	-6.656415	2.321156	1.222014
21.C	-5.631133	2.105989	2.131902
22.C	-4.341119	2.512797	1.837120
23.H	-3.557635	-3.434896	-0.030362
24.H	-4.230135	-2.340810	1.192296
25.H	-2.664438	4.110441	-0.667476
26.H	-2.304141	4.292873	1.069425
27.H	-4.798229	0.143775	-0.048081
28.H	-6.432661	0.954413	-1.699338
29.H	-7.332460	-0.585134	-3.447041
30.H	-6.572619	-2.951182	-3.504819
31.H	-4.923378	-3.763304	-1.838848
32.H	-4.868152	3.834574	-1.236231
33.H	-7.186132	3.130412	-0.702139
34.H	-7.675583	2.000133	1.455671
35.H	-5.839986	1.615827	3.087262
36.H	-3.525758	2.336220	2.549996
37.S	2.162553	0.809085	1.644804
38.S	0.841421	-2.148563	1.659921
39.S	1.579099	1.677986	-1.201531
40.S	1.693879	-1.568707	-1.195281
41.C	2.493975	1.615868	0.207416
42.C	1.707856	-2.429906	0.241937
43.C	3.786900	2.376081	0.182077
44.C	2.662375	-3.586102	0.300922
45.C	4.764056	1.869729	-0.836420
46.H	3.557635	3.434896	-0.030362
47.H	4.230135	2.340810	1.192296
48.C	4.058525	-3.137460	0.627641
49.H	2.664438	-4.110441	-0.667476
50.H	2.304141	-4.292873	1.069425
51.C	5.192383	0.546668	-0.808590
52.C	5.265331	2.722210	-1.810980
53.C	5.088255	-3.344885	-0.280773
54.C	4.341119	-2.512797	1.837120
55.C	6.109088	0.091250	-1.740781
56.H	4.798229	-0.143775	-0.048081
57.C	6.185605	2.267471	-2.742936
58.H	4.923378	3.763304	-1.838848
59.C	6.381825	-2.945644	0.016216
60.H	4.868152	-3.834574	-1.236231
61.C	5.631133	-2.105989	2.131902
62.H	3.525758	-2.336220	2.549996
63.C	6.609120	0.948584	-2.710077
64.H	6.432661	-0.954413	-1.699338

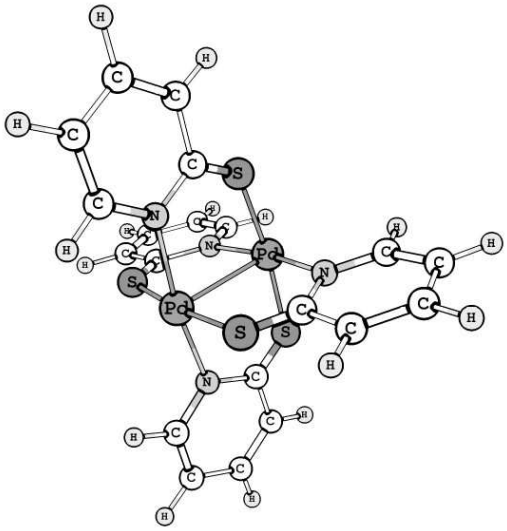
65.H	6.572619	2.951182	-3.504819
66.C	6.656415	-2.321156	1.222014
67.H	7.186132	-3.130412	-0.702139
68.H	5.839986	-1.615827	3.087262
69.H	7.332460	0.585134	-3.447041
70.H	7.675583	-2.000133	1.455671



Compound f

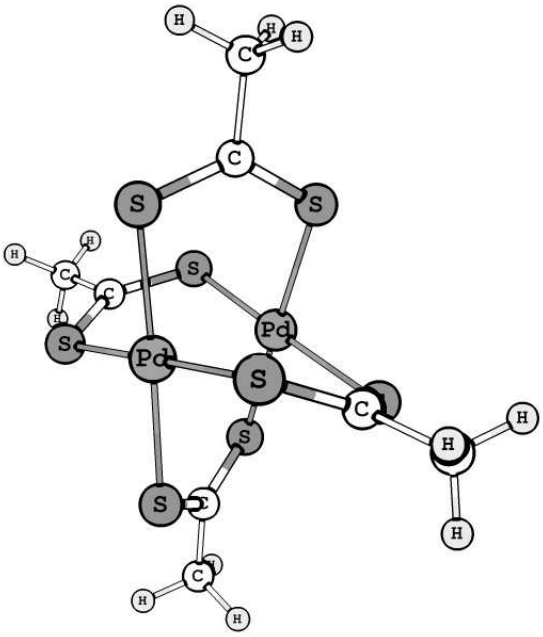
Atom	X	Y	Z (Angstrom)
1.Pd	1.318882	0.018442	-0.004188
2.Pd	-1.318882	-0.018442	-0.004188
3.S	-1.359885	1.734423	-1.513117
4.S	1.359885	-1.734423	-1.513117
5.S	-1.312218	-1.775636	1.500981
6.S	1.312218	1.775636	1.500981
7.N	1.349786	1.356298	-1.514685
8.N	-1.349786	-1.356298	-1.514685
9.N	1.383676	-1.312507	1.510915
10.N	-1.383676	1.312507	1.510915
11.C	0.266431	1.990334	-2.020918
12.C	0.457512	2.954747	-3.028915
13.C	1.710500	3.256418	-3.488127
14.C	2.809111	2.582263	-2.955973
15.C	2.575375	1.646549	-1.982469
16.C	-0.266431	-1.990334	-2.020918
17.C	-0.457512	-2.954747	-3.028915
18.C	-1.710500	-3.256418	-3.488127
19.C	-2.809111	-2.582263	-2.955973
20.C	-2.575375	-1.646549	-1.982469
21.C	0.319000	-1.976144	2.018508
22.C	0.536194	-2.924453	3.036253
23.C	1.795971	-3.179781	3.505095
24.C	2.874574	-2.474562	2.972396
25.C	2.615533	-1.556958	1.988063
26.C	-0.319000	1.976144	2.018508
27.C	-0.536194	2.924453	3.036253
28.C	-1.795971	3.179781	3.505095
29.C	-2.874574	2.474562	2.972396
30.C	-2.615533	1.556958	1.988063
31.H	3.899374	-2.633963	3.313289
32.H	1.947456	-3.924603	4.292372
33.H	-0.338399	-3.446839	3.434077
34.H	-0.431679	3.452821	-3.425540
35.H	1.841334	4.014289	-4.266581
36.H	3.829992	2.779742	-3.288599

37.H	0.431679	-3.452821	-3.425540
38.H	-1.841334	-4.014289	-4.266581
39.H	-3.829992	-2.779742	-3.288599
40.H	0.338399	3.446839	3.434077
41.H	-1.947456	3.924603	4.292372
42.H	-3.899374	2.633963	3.313289
43.H	-3.413624	0.966630	1.530045
44.H	-3.390549	-1.079226	-1.525323
45.H	3.390549	1.079226	-1.525323
46.H	3.413624	-0.966630	1.530045



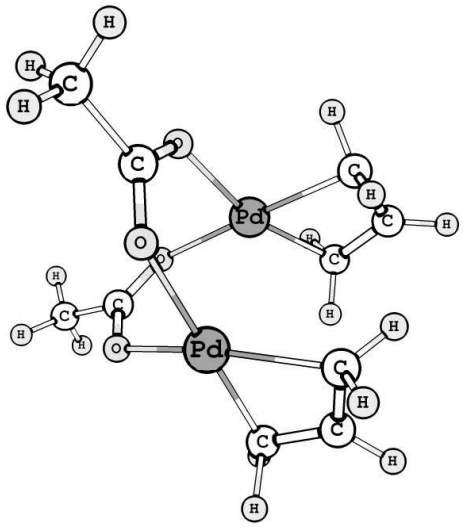
Compound g

Atom	X	Y	Z (Angstrom)
1.Pd	-0.501075	-1.249450	0.002655
2.Pd	0.501075	1.249450	0.002655
3.S	-2.336510	-0.617680	1.250175
4.S	-0.617859	1.788151	1.941511
5.C	-1.953354	0.779441	2.105559
6.S	-1.690386	-0.874610	-1.939425
7.S	1.270245	-2.048232	-1.233328
8.S	0.617859	-1.788151	1.941511
9.S	-1.270245	2.048232	-1.233328
10.S	1.690386	0.874610	-1.939425
11.S	2.336510	0.617680	1.250175
12.C	-1.952973	0.779450	-2.100579
13.C	1.952973	-0.779450	-2.100579
14.C	1.953354	-0.779441	2.105559
15.C	2.903145	-1.182914	-3.175525
16.H	2.418575	-1.056669	-4.158388
17.H	3.805047	-0.552925	-3.163580
18.H	3.186309	-2.240852	-3.071942
19.C	2.943805	-1.199873	3.136463
20.H	3.829434	-1.629164	2.638391
21.H	3.279694	-0.341014	3.736306
22.H	2.519580	-1.971618	3.795634
23.C	-2.943805	1.199873	3.136463
24.H	-3.829434	1.629164	2.638391
25.H	-3.279694	0.341014	3.736306
26.H	-2.519580	1.971618	3.795634
27.C	-2.903145	1.182914	-3.175525
28.H	-2.418575	1.056669	-4.158388
29.H	-3.805047	0.552925	-3.163580
30.H	-3.186309	2.240852	-3.071942



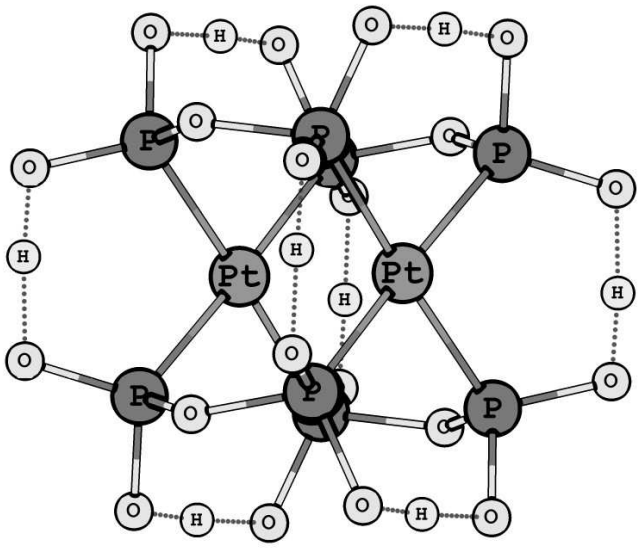
Compound h

Atom	X	Y	Z (Angstrom)
1.Pd	-0.241391	1.209384	0.782951
2.Pd	-0.180446	-1.198104	-0.766736
3.O	0.987196	0.105674	1.995307
4.O	1.411503	-1.527232	0.490925
5.O	1.389817	1.659366	-0.379055
6.O	1.000408	0.039115	-1.909852
7.C	-1.590072	2.611297	0.006913
8.C	-1.374273	-2.790937	-0.133494
9.C	1.614170	-0.906405	1.572347
10.C	2.706166	-1.438956	2.442581
11.H	2.903691	-0.760680	3.282034
12.H	3.615498	-1.583954	1.840214
13.H	2.411055	-2.428889	2.825827
14.C	1.610773	1.054260	-1.466915
15.C	2.686262	1.613075	-2.340582
16.H	3.271743	0.797196	-2.788016
17.H	3.330038	2.298147	-1.773780
18.H	2.212823	2.170837	-3.165559
19.C	-2.159795	-1.822451	-0.787097
20.C	-1.779031	-1.444710	-2.090426
21.H	-2.226945	-0.557683	-2.548589
22.H	-1.387468	-2.195895	-2.787402
23.H	-0.949793	-3.629190	-0.699328
24.H	-1.506939	-2.955357	0.939936
25.H	-2.870605	-1.215713	-0.212913
26.C	-2.279467	1.511804	0.544911
27.C	-2.016340	1.169982	1.887765
28.H	-2.784389	0.804647	-0.125698
29.H	-2.360777	0.207760	2.277836
30.H	-1.865467	1.960678	2.633139
31.H	-1.385313	3.490840	0.630958
32.H	-1.602146	2.780485	-1.074079



Compound Pt-pop

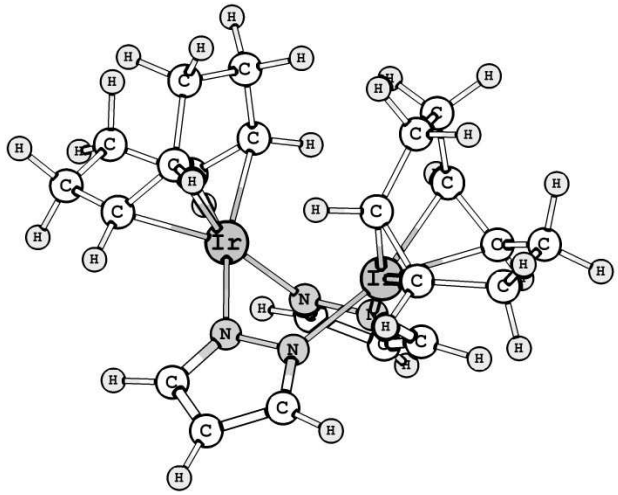
Atom	X	Y	Z (Angstrom)
1.Pt	1.344705	-0.432943	0.152621
2.P	2.076525	1.006043	-1.522572
3.P	1.040940	-2.165667	-1.386568
4.P	0.730669	-1.932427	1.827031
5.P	1.798215	1.244792	1.695919
6.O	2.471138	0.367008	-2.873936
7.O	3.264581	1.944377	-1.073902
8.H	3.180497	2.084155	0.048679
9.O	-0.553120	-2.321185	-1.805023
10.O	1.768566	-1.962412	-2.768313
11.H	2.098618	-0.879022	-2.859224
12.O	1.391535	-3.584411	-0.873656
13.O	1.191276	-3.420350	1.561339
14.H	1.289588	-3.552040	0.445090
15.O	1.163006	-1.559840	3.263294
16.O	0.914242	2.132703	-1.868633
17.O	3.001194	2.158205	1.351288
18.O	1.989615	0.739122	3.178420
19.H	1.601369	-0.315675	3.256278
20.Pt	-1.344385	0.433054	-0.152563
21.P	-2.076768	-1.006024	1.522922
22.O	-2.478207	-0.364435	2.871381
23.O	-3.261869	-1.947922	1.074362
24.H	-3.180811	-2.084046	-0.048905
25.O	-0.911656	-2.130550	1.870640
26.P	-0.728137	1.931821	-1.827290
27.P	-1.042821	2.165489	1.386401
28.O	0.550050	2.318460	1.809400
29.P	-1.798675	-1.244105	-1.695830
30.O	-3.004497	-2.153694	-1.351301
31.O	-1.987144	-0.740706	-3.179419
32.H	-1.598504	0.314117	-3.257327
33.O	-1.773823	1.964150	2.766826
34.H	-2.104387	0.881534	2.857351
35.O	-1.391255	3.584552	0.872584
36.O	-1.190202	3.419401	-1.562055
37.H	-1.289245	3.550941	-0.445396
38.O	-1.157122	1.556327	-3.263876



Compound j

Atom	X	Y	Z (Angstrom)
1.Ir	-0.185905	0.010207	1.546019
2.N	-1.205522	1.541593	0.673423
3.C	-1.737286	2.695238	1.099630
4.C	-2.104251	3.458103	0.000436
5.C	1.278157	-1.443125	2.007400
6.C	0.244605	-1.466921	2.972004
7.C	2.646655	-0.877714	2.299802
8.C	0.357627	-0.865337	4.341560
9.H	-1.848501	2.895689	2.163139
10.N	-1.474864	-1.303588	0.671060
11.C	1.436414	1.300995	1.930383
12.C	0.566978	1.284614	3.044616
13.N	-1.206374	1.541125	-0.673551
14.C	-1.738332	2.695088	-1.099114
15.C	2.758634	0.594608	1.908373
16.C	0.925115	0.552358	4.315661
17.N	-1.475077	-1.304415	-0.671751
18.C	-2.300660	-2.268939	1.099246
19.Ir	-0.187042	0.008264	-1.546657
20.H	-1.850312	2.896097	-2.162382
21.C	-2.300692	-2.269965	-1.099252
22.C	-2.858690	-2.905620	0.000274
23.C	1.278607	-1.443257	-2.008040
24.C	1.435184	1.300729	-1.927739
25.C	0.245548	-1.466929	-2.973289
26.C	0.566496	1.285406	-3.042429
27.H	-3.596367	-3.704974	0.000453
28.C	2.646987	-0.876538	-2.298706
29.C	2.757797	0.595312	-1.905280
30.C	0.358614	-0.862885	-4.341891
31.C	0.925645	0.555076	-4.313984
32.H	-2.602812	4.425050	0.000869
33.H	1.237425	-2.215027	1.224827
34.H	-0.484668	-2.286127	2.891674
35.H	3.410328	-1.463202	1.760565
36.H	2.867607	-1.012323	3.374724
37.H	0.964325	-1.515967	5.004562
38.H	-0.655044	-0.842558	4.779609
39.H	1.357314	2.161486	1.248879

40.H	-0.110924	2.142058	3.162340
41.H	3.156433	0.666532	0.882168
42.H	3.491502	1.119163	2.555259
43.H	2.025933	0.530493	4.414910
44.H	0.553294	1.115332	5.187879
45.H	-2.468595	-2.425093	2.162313
46.H	-2.468009	-2.426791	-2.162321
47.H	1.238183	-2.215783	-1.226083
48.H	1.355232	2.160090	-1.244839
49.H	-0.483063	-2.286836	-2.894327
50.H	-0.111583	2.142906	-3.158741
51.H	2.868775	-1.009406	-3.373603
52.H	3.410720	-1.462165	-1.759778
53.H	3.154743	0.666488	-0.878653
54.H	3.490791	1.121138	-2.550960
55.H	-0.654272	-0.839365	-4.779751
56.H	0.965464	-1.512396	-5.006139
57.H	2.026458	0.534254	-4.412853
58.H	0.553602	1.119029	-5.185366



Compound k

Atom	X	Y	Z (Angstrom)
1.Rh	-0.125563	1.476608	1.322813
2.C	-0.829828	1.898338	3.079839
3.N	-1.286016	2.243905	4.095857
4.C	1.696703	1.520388	1.978132
5.N	2.808727	1.471494	2.326121
6.C	0.521718	1.475244	-0.497882
7.N	0.872227	1.482688	-1.611447
8.C	-1.937067	1.346562	0.651927
9.N	-3.018646	1.182672	0.246129
10.Rh	0.126003	-1.479468	1.324489
11.C	0.829623	-1.902567	3.080140
12.C	-1.694131	-1.525083	1.982130
13.C	-0.523199	-1.476125	-0.494704
14.C	1.935389	-1.347648	0.651304
15.N	1.284096	-2.248915	4.096695
16.N	-2.805772	-1.477078	2.331614
17.N	-0.873925	-1.482747	-1.608259
18.N	3.016105	-1.181750	0.243517
19.C	4.140058	1.376043	2.735411
20.H	4.576982	2.379106	2.860074
21.H	4.207026	0.838348	3.693805

22.H	4.729351	0.826485	1.982729
23.C	-1.831550	2.730365	5.287219
24.H	-1.828904	3.832268	5.282576
25.H	-2.869314	2.380404	5.399111
26.H	-1.243063	2.376452	6.147389
27.C	1.831455	-2.726294	5.291002
28.H	2.129055	-1.885596	5.937021
29.H	1.092879	-3.341755	5.827711
30.H	2.717456	-3.345103	5.078534
31.C	-4.138857	-1.364518	2.730298
32.H	-4.416343	-0.300734	2.821681
33.H	-4.798528	-1.850654	1.993716
34.H	-4.292555	-1.850911	3.705794
35.C	-4.303069	0.940182	-0.245330
36.H	-4.825323	1.888848	-0.444825
37.H	-4.247963	0.362404	-1.181166
38.H	-4.889104	0.361863	0.487703
39.C	4.299405	-0.926562	-0.244358
40.H	4.465624	0.161456	-0.320303
41.H	5.058093	-1.363165	0.424168
42.H	4.425830	-1.371398	-1.243653
43.C	-1.266030	-1.490808	-2.948515
44.H	-1.388894	-0.458072	-3.315852
45.H	-0.509704	-2.003281	-3.563878
46.H	-2.224078	-2.020624	-3.066214
47.C	1.269501	1.498406	-2.950301
48.H	1.376145	2.534297	-3.308923
49.H	2.234051	0.980824	-3.069805
50.H	0.519400	0.987108	-3.575398